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Université de Bordeaux

Activity Report 2016

Project-Team MEMPHIS

Modeling Enablers for Multi-Physics and
Interactions

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

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Project-Team MEMPHIS

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- 6.3.1. - Inverse problems
- 6.3.2. - Data assimilation
- 6.3.4. - Model reduction

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- 1.1.9. - Bioinformatics
- 2.2.1. - Cardiovascular and respiratory diseases
- 4.3.2. - Hydro-energy
- 4.3.3. - Wind energy
- 5.2.1. - Road vehicles
- 5.2.3. - Aviation
- 5.2.4. - Aerospace
- 5.5. - Materials
- 8.4. - Security and personal assistance
- 8.4.1. - Crisis management

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2. Overall Objectives

2.1. Multi-physics numerical modeling

We aim at a step change in multi-physics numerical modeling by developing two fundamental enablers:

- **reduced-order models;**
- **hierarchical Cartesian schemes.**

Reduced-order models (ROMs) are simplified mathematical models derived from the full set of PDEs governing the physics of the phenomenon of interest. ROMs can be derived from first principles or be data-driven. With ROMs one trades accuracy for speed and scalability, and counteracts the curse of dimension by significantly reducing the computational complexity. ROMs represent an ideal building block of systems with real-time requirements, like interactive decision support systems that offer the possibility to rapidly explore various alternatives.

Hierarchical Cartesian schemes allow the multi-scale solution of PDEs on non body-fitted meshes with a drastic reduction of the computational setup overhead. These methods are easily parallelizable and they can efficiently be mapped to high-performance computer architectures. They avoid dealing with grid generation, a prohibitive task when the boundaries are moving and the topology is complex and unsteady.

3. Research Program

3.1. Hierarchical Cartesian schemes

We intend to conceive schemes that will simplify the numerical approximation of problems involving complex unsteady objects together with multi-scale physical phenomena. Rather than using extremely optimized but non-scalable algorithms, we adopt robust alternatives that bypass the difficulties linked to grid generation. Even if the mesh problem can be tackled today thanks to powerful mesh generators, it still represents a severe difficulty, in particular when highly complex unsteady geometries need to be dealt with. Industrial experience and common practice shows that mesh generation accounts for about 20% of overall analysis time, whereas creation of a simulation-specific geometry requires about 60%, and only 20% of overall time is actually devoted to analysis. The methods that we develop bypass the generation of tedious geometrical models by automatic implicit geometry representation and hierarchical Cartesian schemes.

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions [55], [47] and boundary conditions are imposed using appropriate interpolation methods [33], [57], [52]. This eliminates the need for boundary conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.

Hierarchical octree grids offer several considerable advantages over classical adaptive mesh refinement for body-fitted meshes, in terms of data management, memory footprint and parallel HPC performance. Typically, when refining unstructured grids, like for example tetrahedral grids, it is necessary to store the whole data tree corresponding to successive subdivisions of the elements and eventually recompute the full connectivity graph. In the linear octree case that we develop, only the tree leaves are stored in a linear array, with a considerable memory advantage. The mapping between the tree leaves and the linear array as well as the connectivity graph is efficiently computed thanks to an appropriate space-filling curve. Concerning parallelization, linear octrees guarantee a natural load balancing thanks to the linear data structure, whereas classical non-structured meshes require sophisticated (and moreover time consuming) tools to achieve proper load distribution (SCOTCH, METIS etc.). Of course, using unfitted hierarchical meshes requires further development and analysis of methods to handle the refinement at level jumps in a consistent and conservative way, accuracy analysis for new finite-volume or finite-difference schemes, efficient reconstructions at the boundaries to recover appropriate accuracy and robustness. These subjects, that are presently virtually absent at Inria, are among the main scientific challenges of our team.

3.2. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the solution of new problem in physics and the prediction of new phenomena thanks to simulation. However, in industrial applications fast on line responses are needed for design and control. For instance, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known a priori. Therefore the aerodynamic and inertial forces are calculated at a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design will experience in service. A simplistic estimate of the number of analyses required would multiply the numbers of conditions to give 10^7 . Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical loads conditions, meaning that approximately 10^5 simulations are required for conventional aircraft configurations. Furthermore these analyses have to be repeated every time that there is an update in the aircraft structure...

Compared to existing approaches for ROMs [44], our interest will be focused on two axis. On the one hand, we start from the consideration that small, highly non-linear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place close to the walls at the scale of a millimeter for computational domains that are of the order of hundreds of meters. In this context our approach is characterized by a multi-scale model where the large scales are described by far field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

A second characterizing feature of our ROM approach is non-linear interpolation. We start from the consideration that dynamical models derived from the projection of the PDE model in the reduced space are neither stable to numerical integration nor robust to parameter variation when hard non-linear multi-scale phenomena are considered.

However, thanks to Proper Orthogonal Decomposition (POD) [48], [56], [36] we can accurately approximate large solution databases using a small base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [50], [34], Dynamic Mode Decomposition [54]) allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between the modes in parameter

space, thanks to ideas relying on optimal transportation [58], [40] that we have started developing in the FP7 project FFAST and H2020 AEROGUST. In the following we precise these ideas on a specific example.

4. Application Domains

4.1. Energy conversion

We consider applications in the domain of wind engineering and sea-wave converters. As an example of application of our methods, we show a recent realization where we model a sea-wave energy converter, see figure 1. In this unsteady example, the full interaction between the rigid floater, air and water is described by a monolithic model, the Newton's law, where physical parameters such as densities, viscosities and rigidity vary across the domain. The appropriate boundary conditions are imposed at interfaces that arbitrarily cross the grid using adapted schemes built thanks to geometrical information computed via level set functions [55]. The background method for fluid structure interface is the volume penalization method [33] where the level set functions is used to improve the degree of accuracy of the method [38] and also to follow the object. The simulations are unsteady, three dimensional, with $O(10^8)$ grid points on 512 CPUs.

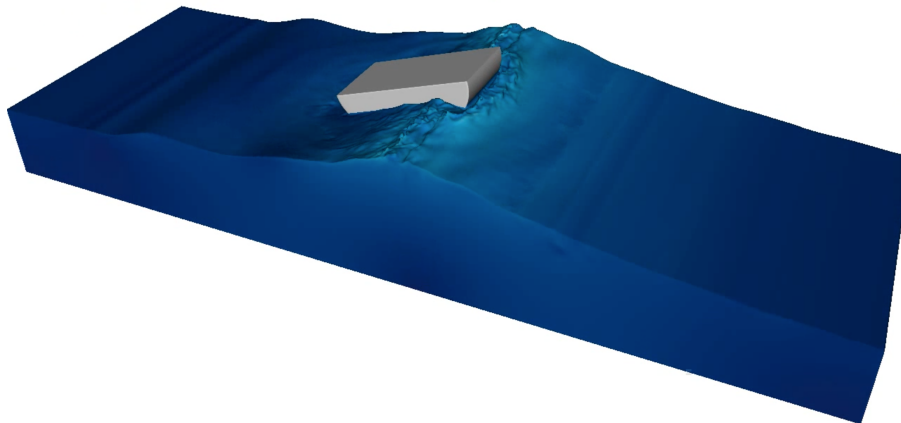


Figure 1. Numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

4.2. Impacts

The numerical modelling of multimaterial rapid dynamics in extreme conditions is an important technological problem for industrial and scientific applications. Experiments are dangerous, need heavy infrastructures and hence are difficult and expensive to realize. The simulation of such phenomena is challenging because they couple large deformations and displacements in solids to strongly non-linear behaviour in fluids. In what follows, we privilege a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws. This approach was introduced in [46] and subsequently pursued and extended for example in [51], [45], [35], [59].

We study hyper-velocity phenomena where several materials are involved. An example of this approach is the impact of a projectile immersed in air over a shield, see figure 2. Using the same set of equations across the entire domain, we model the compressible fluid, the hyperelastic material and the interaction at the interface that models possible rebounds. Only the constitutive laws characterize the different materials.

The simulation is performed over a 4000^2 fixed Cartesian grid so that the resulting numerical scheme allows an efficient parallelization (512 processors in this case) with an isomorphism between grid partitioning and processor topology. The challenge for our team is to increase the accuracy of the simulation thanks to grid refinement in the vicinity of the moving interfaces, still guaranteeing scalability and a simple computational set up.

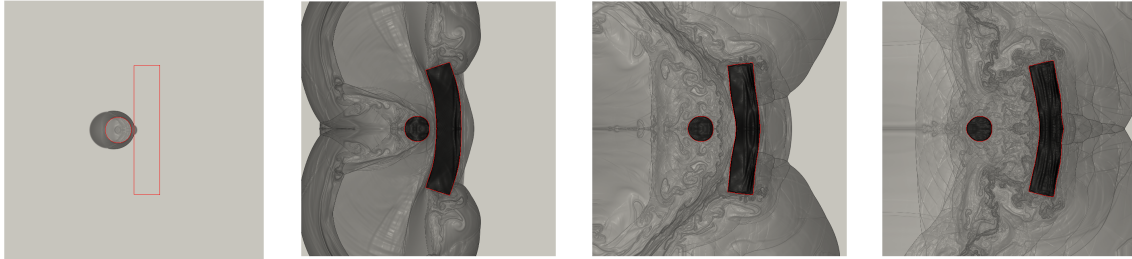


Figure 2. Impact and rebound of a copper projectile on a copper plate. Interface and schlieren at $50\mu s$, $199\mu s$, $398\mu s$ and $710\mu s$. From left to right, top to bottom.

4.3. New materials

Thanks to the multi-scale schemes that we develop, we can characterize new materials from constituents. As an example, consider the material presented in figure 3 left. It is a picture of a dry foam that is used as dielectric material. This micrography is taken at the scale of the dry bubbles, where on the surface of the bubble one can observe the carbon nanotubes as white filaments. The presence of nanotubes in the dry emulsion makes the electrical capacitance of this material significantly affected by its strain state by creating aligned dipoles at a larger scale compared to the size of the dielectric molecules. It is a typical multi-scale phenomenon in presence of widely varying physical properties. This material is used to generate micro currents when it undergoes vibrations. The schemes that we devise allow to model this multi-scale irregular material by a monolithic model (same equation in the whole domain), in this case a variable coefficient diffusion equation. In order to recover adequate accuracy, the numerical scheme is adapted near the interfaces between the different subdomains. The computational hierarchical mesh is directly derived by the micrography of the material (figure 3 right).

4.4. Bio-inspired robotic swimming

In bioinspired robotic swimming the aim is of simulating a three-dimensional swimmer starting from pictures. The first step is to build the three-dimensional fish profile based on two-dimensional data retrieved from the picture of an undeformed fish at rest. This is done by a skeleton technique and a three-dimensional level set function describing the body surface. Then the skeleton is deformed using an appropriate swimming law to obtain a sequence of level set functions corresponding to snapshots of the body surface uniformly taken at different instants.

Thanks to skeleton deformation we typically reconstruct 20% of the snapshots necessary to simulate a swimming stroke, since the time scale of the simulation is significantly smaller than the time step between two subsequent reconstructed snapshots. Also, the surface deformation velocity is required to set the boundary conditions of the flow problem. For this reason it is necessary to build intermediate level set functions and to compute the deformation velocity field between subsequent fish snapshots. Optimal transportation is well suited to achieve this goal providing an objective model to compute intermediate geometries and deformation velocities.

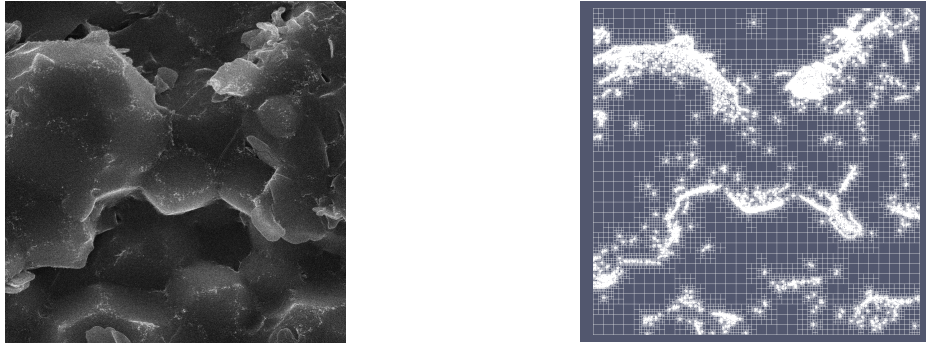


Figure 3. A micrography of an electrostrictive material is shown on the left: the bright regions visualize the carbon nanotubes. The hierarchical grid adapted to the nanotubes is shown on the right. The ratio between the largest and the smallest cell side is 2^7 . Project developed in collaboration with the CRPP physics and chemistry lab of the CNRS in Bordeaux (Annie Colin, Philippe Poulin).

Numerical simulations have been performed in 3D, see figure 4. However, it has been observed that these algorithms do not preserve the physics/features of the represented objects. Indeed, the fish tends to compress during the deformation.

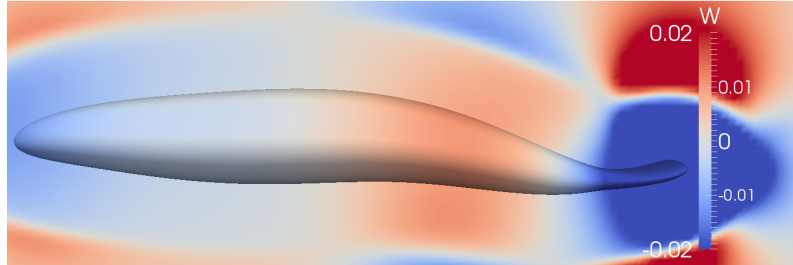


Figure 4. Comparison of the exact deformation velocity (presented inside the swimmer) and the approximated velocity identified using optimal transport (represented outside the fish). The error of the identification scheme is negligible for this component of the velocity, as it can be inferred by comparing the two velocities on the boundary of the swimmer.

For this reason, we will consider incompressible or rigid transports. Another example of bio-inspired swimming is presented in the highlights section.

5. Highlights of the Year

5.1. Highlights of the Year

Numerical simulation of zebrafish larvae C-bend

This part is performed in collaboration with the MRGM laboratory (Laboratoire Maladies Rares : Génétique et Métabolisme, <https://mrgm.u-bordeaux.fr/>). They are interested in the swimming of a zebrafish larvae under genetic modifications. One aim is to quantify the power spent by such fishes to swim after a stimuli reaction. The numerical simulation we develop can help computing integral quantities such the power [39]. This simulation is challenging due to coupling several methods like image treatment (from movies given by MRGM), optimal transport [58] and numerical simulations.

First 2D numerical results have been performed from a series of 615 pictures obtained at a rate equal to 15 000 images per second. The fish is a 8-day zebrafish larvae (length is $\ell = 7\text{ mm}$) presented in figure 5.

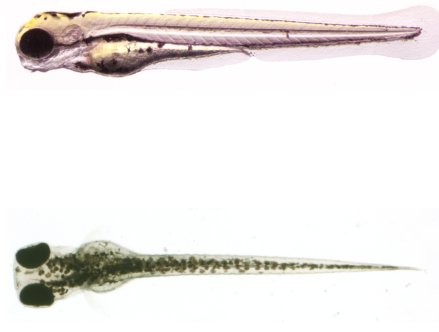


Figure 5. Pictures of a 8-day zebrafish larvae. Source: MRGM.

All the 615 pictures have been post-processed to remove the displacement of the center of mass (due to the hydrodynamic forces) as well as the rotation angle (due to the hydrodynamic torques) to isolate the kinematic of the deformation. Indeed, the displacement of the mass center and the rotation angle have to be computed as being the results of the flow effects generated by the fish deformation. The numerical solver requires however more than 615 images for the overall simulation due to small times steps limitation. The missing images are thus computed using optimal transportation with the algorithm presented in [40]. This method gives also the deformation velocity inside the body that is necessary for our numerical simulation based on the penalty method (see figure 4 for an example of deformation velocity computation).

A comparison between experimental and numerical swimming behaviors is presented in figure 6. The qualitative behaviors look quite similar. In a more quantitative way, figures 7 and 8 show the temporal evolution of the rotating angle as well as the position of the center of mass. The numerical results (displacement of the mass center and the rotation) are quite close to the experimental ones (the ones removed in the post-processed of the original pictures).

The small differences can be explained by the fact the the actual simulation is only two-dimensional. Another explanation is that the deformation velocity obtained by optimal transportation is by definition irrotational and *a priori* non divergence free. We are now working on the 3D simulation as well as a modified (sub-)optimal transportation including rotational effects for a divergence free field.

6. New Software and Platforms

6.1. COCOFLOW

FUNCTIONAL DESCRIPTION

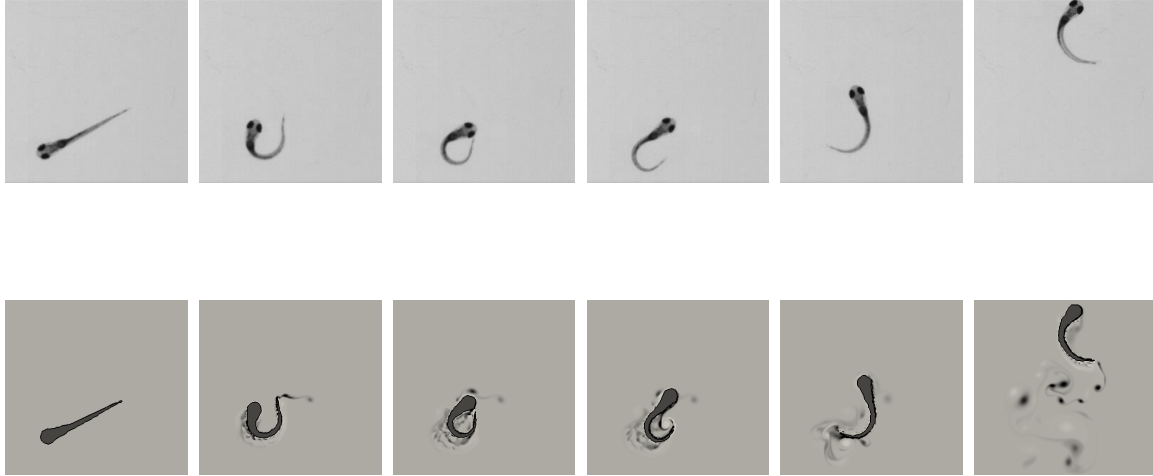


Figure 6. Comparison between experimental (top) and numerical results (bottom) at t_0 , $t_0 + 0.7$ ms, $t_0 + 1.1$ ms, $t_0 + 1.3$ ms, $t_0 + 2$ ms and $t_0 + 4.1$ ms from left to right. Experiments results given by MRGM.

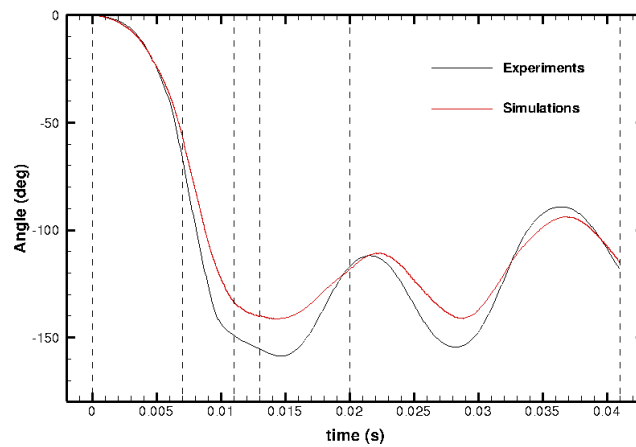
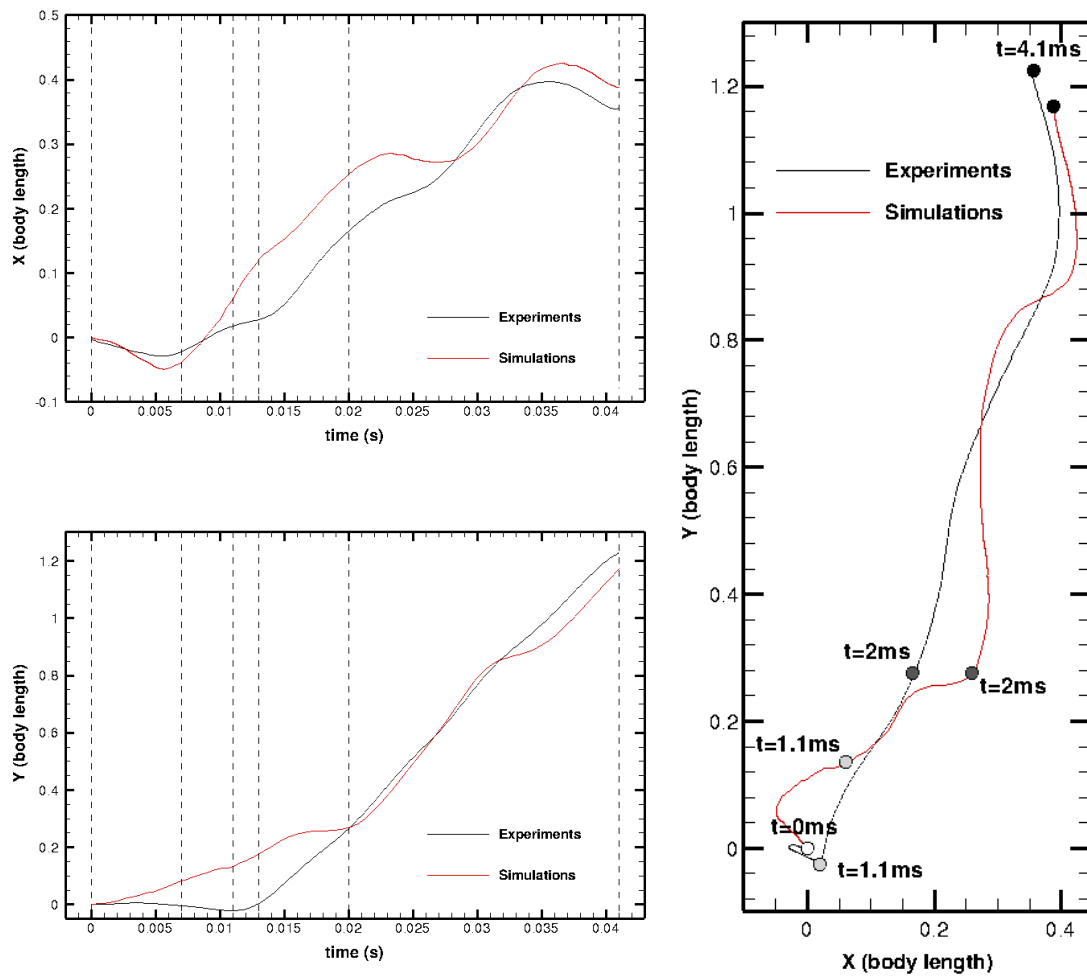


Figure 7. Temporal evolution of the rotation angle.



(a) Temporal evolution of the center of mass.

(b) Position of the center of mass.

Figure 8. Kinematic results for the zebrafish swimming.

The code is written in fortran 95 with a MPI parallelization. It solves equations of conservation modeling 3D compressible flows with elastic models as equation of state.

- Contact: Florian Bernard
- URL: <https://gforge.inria.fr/projects/cocoflow>

6.2. KOPPA

Kinetic Octree Parallel PolyAtomic
FUNCTIONAL DESCRIPTION

KOPPA is a C++/MPI numerical code solving a large range of rarefied flows from external to internal flows in 1D, 2D or 3D. Different kind of geometries can be treated such as moving geometries coming from CAO files or analytical geometries. The models can be solved on Octree grids with dynamic refinement.

- Participant: Florian Bernard
- Contact: Florian Bernard
- URL: <https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary>

6.3. NS-penal

Navier-Stokes-penalization
KEYWORDS: 3D - Incompressible flows - 2D
FUNCTIONAL DESCRIPTION

The software can be used as a black box with the help of a data file if the obstacle is already proposed. For new geometries the user has to define them. It can be used with several boundary conditions (Dirichlet, Neumann, periodic) and for a wide range of Reynolds numbers.

- Partner: Université de Bordeaux
- Contact: Charles-Henri Bruneau

6.4. NaSCar

Navier-Stokes Cartesian
KEYWORDS: HPC - Numerical analyse - Fluid mechanics - Langage C - PETSc
SCIENTIFIC DESCRIPTION

NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

FUNCTIONAL DESCRIPTION

This code is devoted to solve 3D-flows in around moving and deformable bodies. The incompressible Navier-Stokes equations are solved on fixed grids, and the bodies are taken into account thanks to penalization and/or immersed boundary methods. The interface between the fluid and the bodies is tracked with a level set function or in a Lagrangian way. The numerical code is fully second order (time and space). The numerical method is based on projection schemes of Chorin-Temam's type. The code is written in C language and use Petsc library for the resolution of large linear systems in parallel.

NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

- Participant: Michel Bergmann
- Contact: Michel Bergmann
- URL: <https://gforge.inria.fr/projects/nascar/>

7. New Results

7.1. Hybrid POD/DNS: application to aeroelastic windturbine blade

Some new techniques related to Reduced Order Modelling have been developed in the framework of the EU project AEROGUST. The first proposed approach is based on a domain decomposition method in which a POD [56], [43], [44], [37], [36] model is dynamically coupled with a CFD solver [39], [38]. This tool can be used to perform predictive simulations thanks to the fact that the non-linear effects related to new working conditions are directly captured by the CFD solver while the far field region can be efficiently described by the POD model. The hybrid technique has been extended to gust simulations by the introduction of forcing terms which can describe perturbations coming from the far field.

The domain decomposition approach has been proposed also inside an iterative procedure named "numerical zoom" which is based on the use of several mesh levels. This procedure is repeated several times in order to focus the degrees of freedom of the discretisation in the region close to the body.

Finally, the POD method has been proposed also for the acceleration of CFD solver for incompressible flows. The solution of the Poisson problem on the pressure variable which appears in incompressible solvers can be quite time consuming. The proposed approach consists in searching the solution of the Poisson problem in the space spanned by the POD basis. This is done by substituting the POD expansion in the Poisson equation and minimizing the residuals. The robustness of the method has been improved by introducing a check on the quality of the Poisson solution (based on the divergence of the velocity field at the end of the correction step) and a dynamic update of the POD basis.

The domain decomposition approach with the forcing terms has been used to simulate the effects of a gust on a wind turbine blade in a simplified configuration at low Reynolds number. The numerical zoom procedure is applied by coupling a DNS simulation with a POD description of the far field. The solution obtained on three levels of mesh is reported in Figure 9 in which the vortex structures are shown according to the q -criterion. The bending of the blade is described by a non-linear beam model. Figure 10 shows the shapes of the blade without loads, in the chosen working condition and during the gust.

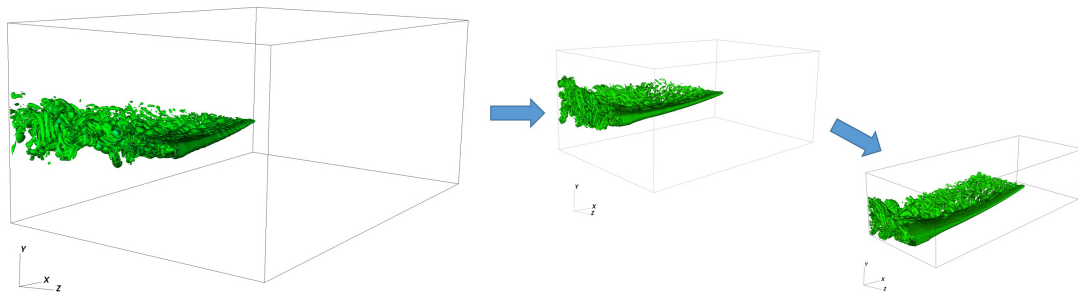


Figure 9. Numerical zoom on the wind turbine blade simulation (vortex structure visualised by q -criterion)

7.2. Discretization of the Laplacian operator using a multitude of overlapping cartesian grids

A new finite-difference approach to solve a Laplacian operator has been developed, using patches of overlapping grids where a fined level is needed, leaving coarser meshes in the rest of the computational domain. These overlapping grids will have generic quadrilateral shapes (as shown in figure 11).



Figure 10. Blade shape without loads (top), in the chosen working condition (middle) and during the gust (bottom)

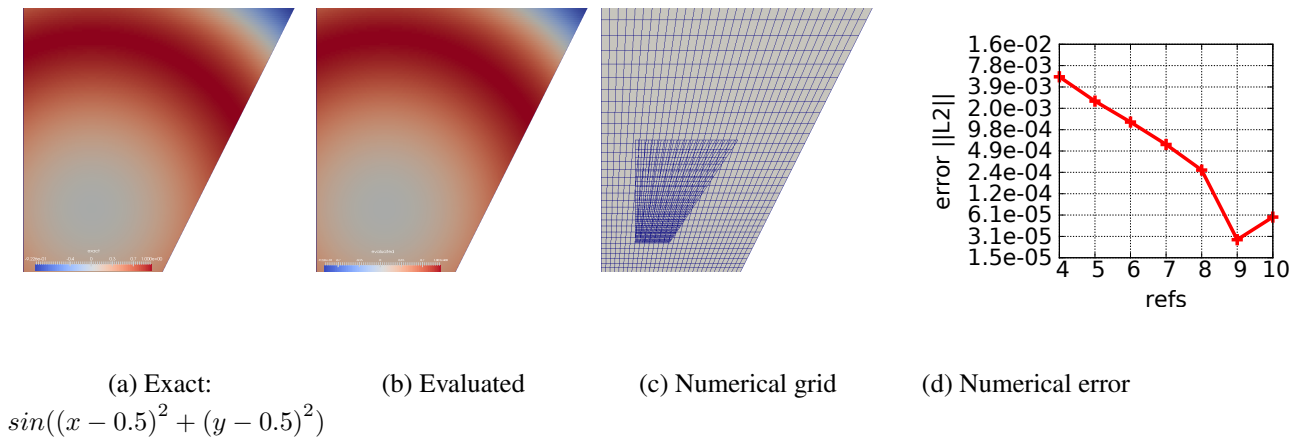
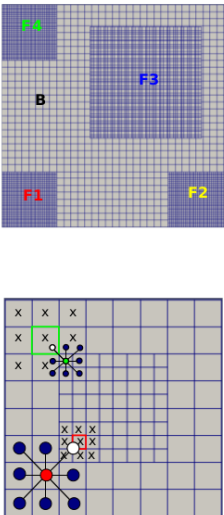


Figure 11. results

A monolithic approach is used to solve the algebraic equations, applying restriction and prolongation operators to fill the non-diagonal blocks of the resulting matrix. These operators work on data structures communicated between the different grids using ad hoc parallel inter-communicators, as shown in figure 12. 12.



$$\begin{bmatrix} D & R & R & R & R \\ P & D & 0 & 0 & 0 \\ P & 0 & D & 0 & 0 \\ P & 0 & 0 & D & 0 \\ P & 0 & 0 & 0 & D \end{bmatrix} \times \begin{bmatrix} x \\ x \\ x \\ x \\ x \end{bmatrix} = \begin{bmatrix} f \\ f \\ f \\ f \\ f \end{bmatrix}$$

Blocks D are the discretization matrices onto each grid
(parallel intra-communications).

Blocks R and P are the restriction and prolongation operators between the grids
(parallel inter-communications).

Figure 12. Monolithic approach

Works are going on to change the solver from the finite-difference approach to a finite-volume one, and to implement the 3D case. The use of a finite-volume solver can benefit from the usage of octree patches instead of cartesian grids, obtaining a more accurate refining and a greater precision.

7.3. Numerical simulation of a biomimetic LVAD developed by CorWave

We just started a collaboration with the PME CorWave. The CorWave LVAD utilizes an undulating disc wave pumping mechanism, replacing the high speed, high shear impeller of current continuous flow rotary pumps. Louis de Lillers, the CorWave project manager, has contacted MEMPHIS to perform numerical simulations and optimizations of their LVAD. This collaboration has started with an industrial PhD (Cifre, Antoine Fondaneche). Figure 13 shows preliminary results (proof of concept) for the CorWave LVAD obtained with the code NaSCar described in [38].

7.4. A sharp Cartesian method for incompressible flows with large density ratios

We have developed and validated a new Cartesian method for bifluid incompressible flows with high density ratios. The specificity of the method relies on a sharp second order numerical scheme for the spatial resolution of the discontinuous elliptic problem for the pressure, that was developed in [42]. The Navier-Stokes equations are integrated in time thanks to a fractional step method based on the Chorin scheme and discretized in space on a Cartesian mesh. The bifluid interface is implicitly represented using a level set function. The numerical tests show the improvements due to this sharp method compared to classical first order methods. As an illustration, we present here numerical results for the dam break test case.

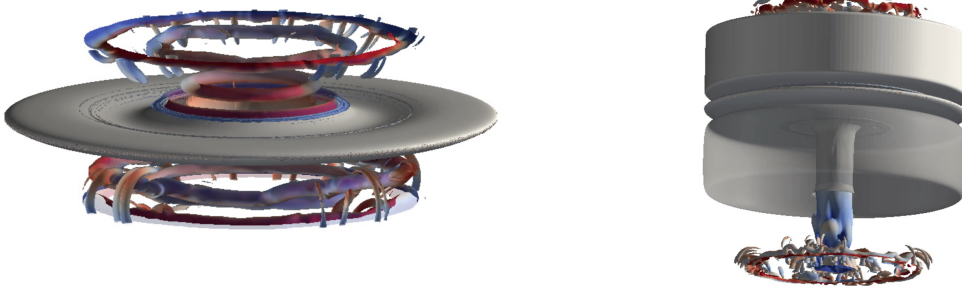


Figure 13. Preliminary results (proof of concept) for the CorWave LVAD. Left: oscillating membrane, right: the whole pump system.

This test case is studied in [53] and [41], and based on experiments conducted in [49]. The initial configuration is a water column at rest in air. The initial height and width of the column are both 5.715 cm. The domain size is 40 cm \times 10 cm. The value of the physical parameters are

$$\left\{ \begin{array}{l} \rho_{water} = 1000 \text{ kg/m}^3, \\ \mu_{water} = 1.137 \times 10^{-3} \text{ kg/ms}, \\ \rho_{air} = 1.226 \text{ kg/m}^3, \\ \mu_{air} = 1.78 \times 10^{-5} \text{ kg/ms}, \\ \sigma = 0.0728 \text{ kg/s}^2 \\ g = -9.8 \text{ m/s}^2 \end{array} \right. \quad (1)$$

We present in Figure 14 the interface evolution at non-dimensional times $T = t\sqrt{g/h} = 0, 1, 2, 3, 4$, with h the initial height of the water column. The computations are performed with 256×64 points.

In Figure 15, we plot the evolution in time of the water front, compared to the experimental results of [49], and to the results obtained for the Ghost-Fluid method and the conservative method of Raessi and Pitsch [53]. We observe that the front propagation is in agreement with the experimental results and the results of the conservative method presented in [53]. It means that, though the method is not strictly conservative, the numerical errors due to momentum transfer across the interface are not large enough to slow down the propagation of the front. It is not the case for instance for the Ghost-Fluid method, as it can be noticed in Figure 15 and has been reported in [53].

7.5. Platooning of trucks on highways

In the context of energy saving, the platooning of ground vehicles on top of a road, in particular highways has been studied. The numerical simulations are performed in 2D and 3D for up to 10 billions unknowns on 384 cores. The goal is to have trucks autonomously following their leader to form a road train in order to improve traffic flow efficiency and to reduce oil consumption. Thus the distance between trucks is short. For instance a gain of about 40% can be obtained on the drag coefficient of the followers when the distance between trucks is equal to 1.8125 their height (see the figure 16), that is approximately eight meters. Even the leader has a lower drag coefficient (-10%) as the first follower compresses the flow in its wake. In the figure it is clearly shown that the pressure gradients inside the gap between the vehicles are much lower than in front of the leader.

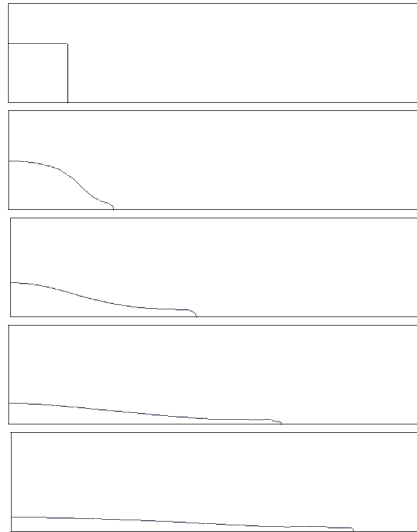


Figure 14. Evolution of the interface for the dam break problem at non-dimensional times $T = t\sqrt{g/h} = 0, 1, 2, 3, 4$.

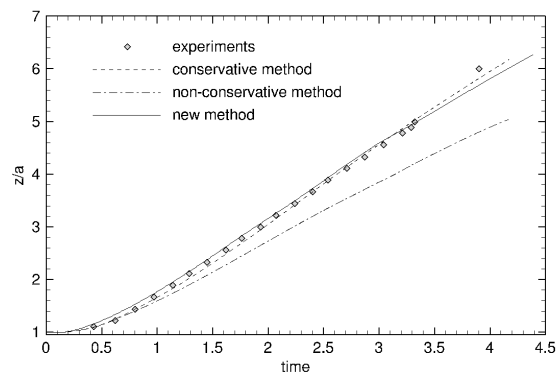


Figure 15. Evolution of the front of propagation: comparison between experimental data and several numerical methods: the Ghost Fluid method (non-conservative method), the conservative method of Raessi and Pitsch and our new method, The dimensionless location of the front $\frac{z}{a}$ is plotted as a function of the dimensionless time $t\sqrt{qh}$.

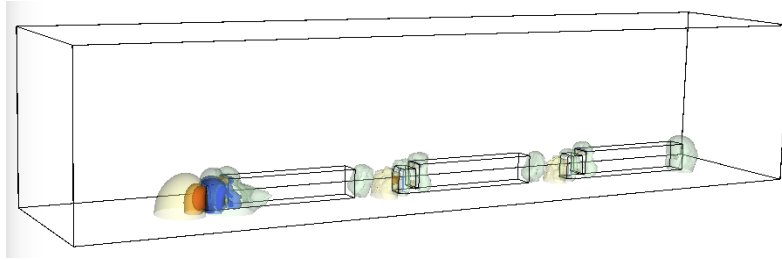


Figure 16. Mean pressure contours of the mean flow around three simplified European tractor-trailer geometries with a distance equal to 1.8125 their height on top of a road in three dimensions.

7.6. Non-linear elasto-plastic dynamics of compressible materials

We describe a numerical model to simulate the non-linear elasto-plastic dynamics of compressible materials. The model is fully Eulerian and it is discretized on a fixed Cartesian mesh. The hyperelastic constitutive law considered is neo-hookean and the plasticity model is based on a multiplicative decomposition of the inverse deformation tensor. The model is thermodynamically consistent and it is shown to be stable in the sense that the norm of the deviatoric stress tensor beyond yield is non increasing. The multimaterial integration scheme is based on a simple numerical flux function that keeps the interfaces sharp. Numerical illustrations in one to three space dimensions of high-speed multimaterial impacts in air are presented.

In TC4 an iron sphere is impacting an aluminium plate immersed in air. The computational domain is $[-0.3, 0.7] \times [-0.4, 0.4] \times [-0.4, 0.4]$ m. The initial velocity of the projectile is $1000m.s^{-1}$. The computation is performed on a $500 \times 400 \times 400$ mesh with 216 processors. Homogeneous Neumann conditions are imposed on the left and right borders and cantilever on the others.

The results are given in Fig 17 where we present the Schlieren results on the vertical symmetry plane and the material interfaces. As in the 2D case the projectile perforates the aluminium plate which is strongly stretched. The breaking of the plate at final time is due to the level set function resolution.

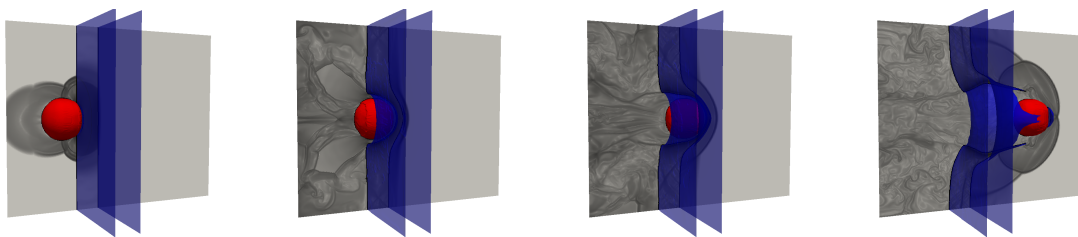
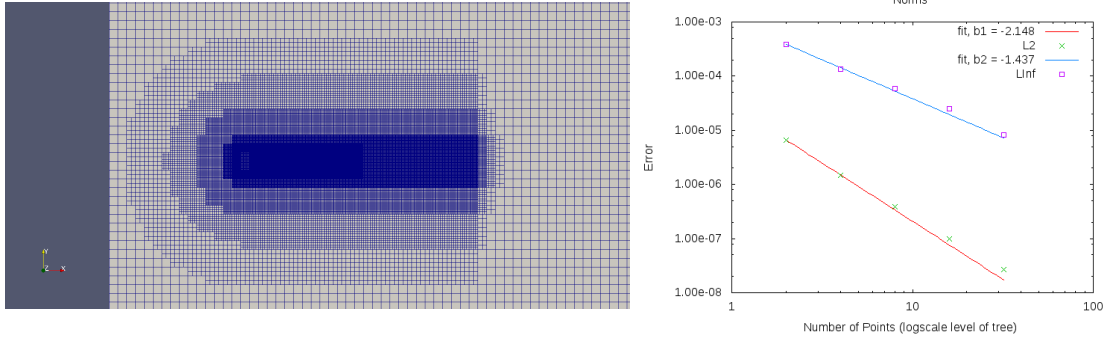


Figure 17. Schlieren representation on the vertical symmetry plane and the material interfaces.

7.7. Hierarchical grids: applications with quadtrees/octrees

A first application with a specific method is the resolution of the incompressible Navier-Stokes equations. A Navier-Stokes solver dealing with quadtrees has been implemented in parallel this year. The overall aim will be to model in 3D the flow over a wind turbine using an Octree grid. On the figure 18 can be seen an example of QuadTree mesh. A Finite Volume Semi-Lagrangian scheme is used.



(a) Example of QuadTree mesh for circular cylinder (b) Norms as a function of number of points on grid

Figure 18.

First, the order of convergence of the Laplacian Solver discretization on QuadTrees has been computed and compared with those obtained with other schemes as explained previously. The method for solving the Laplacian Solver is named Diamond method and consists in using a dual mesh and considering that the Gradients are constants inside. The order of convergence of 2 has been obtained. The order of convergence of the overall Navier-Stokes resolution on QuadTree meshes has been computed and the order of 2 is get as can be seen on figures 18. For the L_∞ norm, the order of 2 can't be reach caused by the loss of accuracy when a gap in refinement level occurs.

For now the grid is fixed, so the next step will be to refine and coarsen the grid following the position of the obstacle and the "interesting" areas. The work will then go on with the implementation of this Navier-Stokes solver with adaptive QuadTree meshes in 3D.

A second application is phase changing material. We consider problems governed by linear elliptic equations with discontinuity interfaces across the domain. The equation coefficients, the solution and its normal derivative can undergo a jump across these internal boundaries. We present a compact second-order finite-difference scheme on a tree-based adaptive grid that can be efficiently solved in parallel. The main idea is to optimize the truncation error of the discretization as a function of the local grid configuration.

The variable coefficient heat diffusion problem we consider is modeled by:

$$-\operatorname{div}(\kappa(\vec{x})\nabla u(\vec{x})) = g(\vec{x}), \quad \text{in } D, \quad (2)$$

$$R(\kappa\partial_{\vec{n}}u(\vec{x}))_S = [u], \quad \text{on } \gamma \quad (3)$$

$$[\kappa(\vec{x})\partial_{\vec{n}}u(\vec{x})] = 0, \quad \text{on } \gamma \quad (4)$$

Where $\vec{x} = (x, y, z)$ are the spatial coordinates and $\kappa(\vec{x})$ is piecewise continuous on each subdomain but it may be discontinuous across γ (the boundary of the D subdomain that contains the discontinuities through). A cell-centered investigation often leads to a symmetric linear system, since the relation between two neighbors is reflective. Considering the configuration in Fig. 19 it is natural to define the discretization at c_4 in terms of the others.



Figure 19. A test configuration centered in c_4 .

Let h be the side length of the cell c_4 . To obtain the existence of a linear consistent scheme we must be able to find the coefficients a_i such that:

$$u_{xx} + u_{yy} = a_1u_1 + a_2u_2 + a_3u_3 + a_4u_4 + a_5u_5 + a_6u_6 + a_7u_7 + O(h)$$

A complete Taylor's analysis on all the involved neighbors, applying them relative linear combinations of the expansions, implies that the coefficients a_i must satisfy the following linear system:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -h & 0 & -h & \frac{3h}{2} & -\frac{h}{2} & \frac{3h}{2} \\ 0 & h & h & 0 & \frac{h}{2} & -\frac{3h}{2} & -\frac{3h}{2} \\ 0 & \frac{h^2}{2} & 0 & \frac{h^2}{2} & \frac{9h^2}{8} & \frac{h^2}{8} & \frac{9h^2}{8} \\ 0 & -h^2 & 0 & 0 & \frac{3h^2}{4} & \frac{3h^2}{4} & -\frac{9h^2}{4} \\ 0 & \frac{h^2}{2} & \frac{h^2}{2} & 0 & \frac{h^2}{8} & \frac{9h^2}{8} & \frac{9h^2}{8} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ a_7 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

In the example above there are seven concerned points, so, we can determine infinite solutions of the complete system but we search a unique one. Let M be the constraints matrix, \vec{a} the weights vector, \vec{f} the right hand side vector for consistency and $F(\vec{a})$ a weights function. The problem to minimize has the Lagrangian form:

$$\mathcal{L} = F(\vec{a}) - \vec{\lambda}(M\vec{a} - \vec{f}) \quad (5)$$

We write the minimization problem (5) in matrix form like:

$$Ax = b \Leftrightarrow \begin{cases} \frac{\partial F(\vec{a})}{\partial \vec{a}} - M^T \vec{\lambda} = 0 \\ M\vec{a} = \vec{f} \end{cases}$$

This choice allows us to implement a scheme always consistent case by case.

Following a consistence proof several tests have been produced to strenghten our method like penalization and different kinds of model until a modeling of the problem (7.7) step by step. We built a new cell centered finite difference method able to:

- be consistent and locally convergent to second order on balanced grids;
- simplify and promote an AMR approach along discontinuity;
- solve the coupled problems (2)-(3) and (2)-(4);
- a first consistent result on the complete model (2)-(3)-(4).

The finite different method presented here has been compared with two other methods finite volume scheme (Fig. 20). The first one has been implemented by Marco Cisternino and the diamonds one by Claire Taymans (see previous sections). All the three methods stick on the same grid and they use PABLO's data structure with its parallel balance.

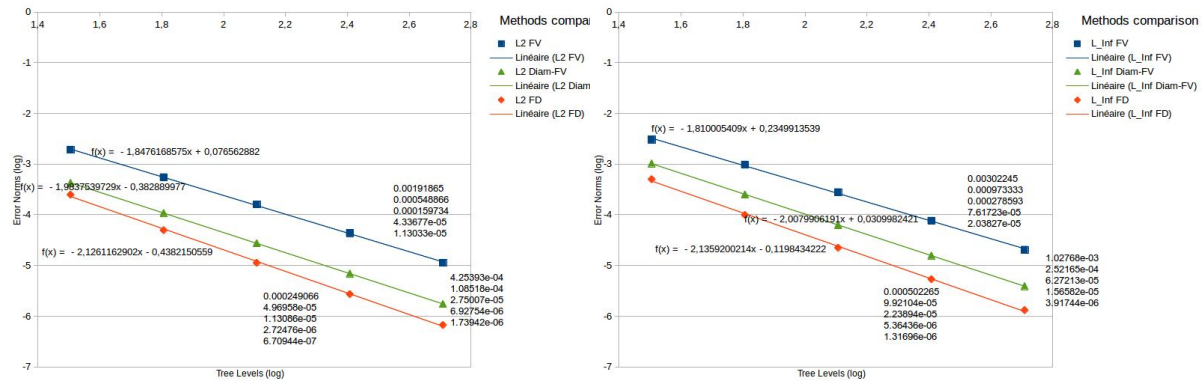
(a) L_2 norm comparison(b) L_∞ norm comparison

Figure 20. Comparison between several numerical approaches.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

We intend to pursue our partnership with Valeol, a wind turbine contractor in Aquitaine. Valeol poses simulation problems that cannot be addressed with standard tools. We have developed for them simplified PDE models for design in the frame of an industry funded PhD (CIFRE). We are currently adapting octree and Chimera approaches to the design of aerodynamic appendices to improve performance of existing installations. This is done in the frame of yet another CIFRE PhD thesis and the corresponding research contract. Moreover, thanks to this technology readiness, Valeol could join for the first time an H2020 research project, AEROGUST, that we are promoting with several academic and industrial institutions across Europe.

This year, we have also developed an new collaboration with the CorWave (<http://www.corwave.fr>). CorWave develops blood pumps based on a unique and patented wave membrane pumping technology. This collaboration has begun with an industry funded PhD (CIFRE), officially for the early 2017. Antoine Fondaneche, the PhD candidate, is now employed by CorWave on a basis of a two-month CDD contract.

We continue to deploy our effort in flow control and drag reduction for ground vehicles. After a fruitful collaboration with Renault, we are in the phase of negotiating a new collaboration. A new collaboration is starting with Valeo to optimize car cooling devices. DNS simulations are performed and compared to the industrial results obtained with URANS and LES methods and an EU network about this subject is going to be proposed.

9. Partnerships and Cooperations

9.1. Regional Initiatives

The project members are actively participating to the CPU cluster of excellence of Idex Bordeaux (<http://cpu.labex.u-bordeaux.fr/>)

9.2. National Initiatives

We belong to the GDR AMORE on ROMs.

9.2.1. Starting grants

A PEPS project ("Programme Exploratoire Premier Soutien"), initiated by Afaf Bouharguane, about Optimal Transport Theory. Angelo Iollo and Lisl Weynans are also involved in this project.

A PEPS project ("Programme Exploratoire Premier Soutien") on the numerical simulation of the biomimetic undulatory swimming for both under water vehicle optimisation and the Modeling of human locomotor system, initiated by Michel Bergmann with the MRGM laboratory (Laboratoire Maladies Rares : Génétique et Métabolism, <https://mrgm.u-bordeaux.fr/>). Afaf Bouharguane and Angelo Iollo are also involved in this project.

NEMO (A Numerical Enabler for MultiPhysics Simulations on Octrees) is an action to improve and merge all the main MEMPHIS numerical codes. To achieve this goal we have a 12 months financial support (Inria BSO FRM) for a young engineer. This work will be done with strong interaction the the local Inria BSO SED as well as Philippe Depouilly from the IMB "SED".

SMecH is a start-up project in software edition, carried on by Florian Bernard, research engineer in the MEMPHIS team. The project aims at porting to an industrial level the numerical codes developed by the MEMPHIS team. The different collaboration with industrial partners have highlighted the need of new numerical tools to simulate high complexity phenomena such as atmospheric reentries, multi-material flows or fund-structure interactions, but also to highly automatize the numerical simulation workflow to save engineer time. The research codes developed in the MEMPHIS team could match perfectly to this need thanks to:

- the various innovative multi-physics models implemented
- the use of Hierarchical Cartesian schemes that automatize the treatment of moving geometry with accuracy
- the development of schemes suitable for High Parallel Computing.

This year, the project has been submitted to the DGD, the Inria department in charge of technological transfert, and has been granted an engineer for 6 months as well as the support of IT-Translation.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

EU research projects were and will be a privileged instrument of diffusion and transfer of our results. The AEROGUST H2020 project involves aeronautical industry (Airbus, Dassault, Piaggio..) and research labs (University of Bristol, DLR, NLR, University of Cape Town) and is dedicated to modeling of aerodynamic gust response for applications. We take part in this project by developing simulation models for unsteady aeroelastic problems and data-driven reduced-order models. We played a similar role for the past in the FP7 project FFAST with the same partners.

9.3.1.1. AEROGUST

Title: Aeroelastic Gust Modelling

Programm: H2020

Duration: May 2015 - April 2018

Coordinator: University of Bristol

Partners:

Airbus Defence and Space (Germany)

University of Cape Town (South Africa)

Dassault Aviation (France)

Deutsches Zentrum für Luft - und Raumfahrt Ev (Germany)

Stichting Nationaal Lucht- en Ruimtevaartlaboratorium (Netherlands)
Numerical Mechanics Applications International (Belgium)
Optimad Engineering S.R.L. (Italy)
Piaggio Aero Industries Spa (Italy)
The University of Liverpool (United Kingdom)
University of Bristol (United Kingdom)
Valeol (France)

Inria contact: Angelo IOLLO and Michel Bergmann

Encounters with atmospheric turbulence are a vitally important in the design and certification of many manmade structures such as aircraft and wind turbines. Gusts cause rapid changes in the flow about the structures which leads to rigid and flexible unsteady responses. Knowledge of aircraft/gust interactions is therefore vital for loads estimation during aircraft design as it impacts on control systems and often defines the maximum loads that these structures will experience in service. At present industry typically uses the linear doublet lattice method with static loads corrections from expensive wind tunnel data. The wind tunnel data is created using the final aerodynamic surface in the predicted cruise shape. This means that gust loads come relatively late when the design options have been narrowed. Increased competition and environmental concerns are likely to lead to the adoption of more flexible materials and the consideration of novel configurations, in which case the linear assumptions of the current gust loads process will become unacceptable. To introduce non-linearity into the gust loads process without significantly increasing the cost and time, this project has three main objectives: to carry out investigations using CFD so that the non-linearities in gust interactions are understood; to create a gust loads process that does not require wind tunnel data and hence reduces the need for wind tunnel testing; to develop updated reduced order models for gust prediction that account for non-linearity at an acceptable cost. These investigations will reduce the need for expensive wind tunnel testing and hence lead to time and cost savings at the design stage therefore ensuring that the European aerospace and defense industry remain competitive in the future. The wind turbine industry has similar concerns, with gusts and wind shear restricting the locations available for wind farms. The project will also address these issues using common methodology.

9.3.2. Collaborations with Major European Organizations

Partner 1: Chalmers University (Sweden)

This activity is complemented by several international interactions, in particular with Chalmers University in order to converge towards the real implementation of new control technologies on cars, buses and trucks.

Partner 2: Optimad Engineering , Torino (Italy)

We have a crucial partnership with Optimad Engineering, a spin-off of the Politecnico di Torino. This society has implemented in industrial codes several schemes that we have developed for the past. In exchange, we have access to these codes. One example is Pablo, an octree managing parallel library (<http://www.optimad.it/products/pablo/>). Three former PhD students at Inria are presently employed in Optimad and several others have spent or will spend a research period in this company in order to get acquainted with code architecture and massive parallelism. This company represents for us an ideal partner for the actual industrial feedback on our methods. As mentioned, we plan to create a local start-up in close collaboration with Optimad. This start-up will respond to actual industrial needs by specific software packages built starting from open source tools that are made available to the applied research community via a consortium. Florian Bernard has been recruited in Memphis for two years with the objective of bringing to a higher maturity level a set of modules developed within the team. He plans to fully invest himself in the creation of the start-up. As for the consortium, we are discussing with several partners including Cineca (Italy HPC center) and Optimad about how to structure such a mutual effort. The Storm Inria team is included in the discussions as a possible partner.

Partner 3: W4E (Wave for Energy) (Italy)

One project is the design of an ISWEC (Inertial Sea Wave Energy Converter) in collaboration with W4E (Wave for Energy), Optimad and others. The ISWEC is a floater prototype that can extract energy from the sea waves. The mechanism is based on a gyroscope that is rotating due to the passive motion of the floater. This prototype is actually tested in the Mediterranean sea in Italy. We will develop the numerical simulation as well as the shape optimization of the ISWEC.

Partner 4: MRGM (Maladies Rares : Génétique et Métabolisme), Bordeaux University (France)

We develop a collaboration with the MRGM lab. They are interested in the swimming of a zebrafish larvae under genetic modifications. One aim is to quantify the power spent by such fishes to swim after a stimuli reaction. The numerical simulation we develop can help computing integral quantities such as the power. This simulation is challenging due to the coupling several methods like image treatment (from movies given by MRGM), optimal transport and numerical simulations.

Partner 5: CRPP (Centre de recherche Paul Pascal), LOF (Laboratoire du Futur) and LOMA (Laboratoire Ondes et Matière d'Aquitaine) labs, Bordeaux University, France.

We established collaborations with physics and chemistry labs in Bordeaux, namely the CRPP, the LOF and the LOMA. They are concerned with the behavior of many passive (CRPP and LOF) and active (LOMA) particles in an incompressible flow. With these partners, we intend to use a combined experimental and computational approach to calibrate models in the case of dilute and concentrated suspensions. The numerical simulations of such particles can help to understand some underlying phenomena at the particles scale and thus to develop mesoscopic models for the whole system (PhD of Baptiste Lambert, oct. 2015).

9.4. International Initiatives

9.4.1. Inria International Labs

9.4.1.1. Declared Inria International Partners

Collaboration with Optimad Engineering.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Giovanni Russo, Professor at the Catane university, has visiting our team several times this year.

Johnny Guzman, associate professor, Université de Brown, USA, one week.

9.5.1.1. Internships

Mohsen Broumand, a PhD visitor from Winnipeg university, has a collaboration with Lisl Weynans for bi-fluid simulations (from October 2016).

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Selection

10.1.1.1. Reviewer

Charles-Henri Bruneau has reviewed several papers for the 9th International Conference on Computational Fluid Dynamics, July 10th-15th, Istanbul.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

Angelo Iollo is in the advisory board of Acta Mechanica.

10.1.2.2. Reviewer - Reviewing Activities

Journal of Computational Physics, International Journal of CFD, Journal of Non-linear Analysis B, ASME Journal of Computational and Nonlinear Dynamics, Journal of Fluid Mechanics, Acta Mechanica, AIAA Journal, International Journal Numerical Methods in Fluids, Computers & Fluids, Journal of Engineering Mathematics, European Journal of Mechanics / B Fluids, Journal Européen de Systèmes Automatisés, Applied Mathematics and Computation. Nuclear Science and Engineering, Computer Methods in Applied Mechanics and Engineering, Journal of Theoretical Biology, Computational Optimization and Applications. Applied science, Meccanica.

10.1.3. Invited Talks

The invited talks are [15], [16], [17], [18].

10.1.4. Leadership within the Scientific Community

Angelo Iollo is responsible of the scientific policy of the scientific computing departement of the LabEx CPU. This department gathers 60 researchers of the math lab IMB, of the computer science lab LaBRI, of the mechanics lab I2M and of the CEA.

10.1.5. Scientific Expertise

Michel Bergmann: reviewer of the PhD defense *Apprentissage d'estimateurs sans modèle avec peu de mesures - Application à la mécanique des fluides* de Kévin Kasper, Ecole normale supérieure de Cachan, 12/10/2016.

Michel Bergmann: member of the Inria Young Researchers Commission, which allocates PhD and Postdoc grants.

Lisl Weynans has participated to the *Comités de sélection* Cnam and Paris 5 Descarte, may 2016.

Angelo Iollo: Président du jury d'HDR de Heloise Beaugendre, Institut de Mathématiques de Bordeaux, université de Bordeaux, mars 2016.

Angelo Iollo: Membre Jury HDR de Laurent Cordier, Institut P', université de Poitiers, novembre 2016.

Angelo Iollo: Membre du Jury de thèse de Loic Lacouture « Modélisation et simulations de mouvement de structures fines » département de mathématiques, juin 2016, Université Paris Sud.

Angelo Iollo: Président du jury de thèse de Olivier Gallinato, « Modélisation du processus cancéreux et méthodes superconvergentes de résolution de problèmes d'interface sur maillage cartésien », Institut de Mathématiques de Bordeaux, université de Bordeaux, novembre 2016.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Four members of the team are Professors or Assistant Professors at Bordeaux University and have a teaching duty, which consists in courses and practical exercises in numerical analysis and scientific computing. Michel Bergmann (CR) also teaches around 64 hours per year (practical exercises in programmation for scientific computing).

10.2.2. Supervision

PhD in progress : Alice Raeli, Numerical Modelling for Phase Changing Materials, 12/06/2014, Azaiez M., Bergmann M., Iollo A.

PhD in progress : Claire Morel, Modélisation aérodynamique 3D d'une turbine éolienne, 01/01/2015, M., Bergmann M., Iollo A.

PhD in progress : Federico Tesser, Identification of dense suspensions rheology, 01/11/2014, Bergmann M., Iollo A.

PhD in progress : Baptiste Lambert, modélisation et simulations numériques des contacts dans des écoulements chargés en particules, 01/10/2015, Bergmann M., Weynans L.,

PhD in progress : Emanuela Abbate, Méthodes numériques pour problèmes stiff en mécanique des fluides et élasticité, 01/11/2015, Iollo, A.

PhD in progress : Mathias Braun, Modèles réduits et problèmes inverses pour l'étude de la résilience des réseaux d'eau potable, 01/10/2015, Iollo A. and Mortazavi I.

PhD in progress : Meriem Jedoua, Introduction d'une méthode efficace de capture d'interface permettant la localisation d'un grand nombre d'objets immergés dans un fluide. Applications à des solides rigides et des vésicules (membranes élastiques) immergés dans un fluide incompressible, 01/10/2013, Bruneau C.-H. and Maitre E.

2012-2016. Dr. Hervé Ung. Ancien ENSEIRB-MATMECA. Problèmes inverses dans les réseaux d'eau potable. Angelo Iollo, Iraj Mortazavi, Bourse Irstea.

10.2.3. Juries

Michel Bergmann has been reviewer of the PhD defense *Apprentissage d'estimateurs sans modèle avec peu de mesures - Application à la mécanique des fluides* de Kévin Kasper, Ecole normale supérieure de Cachan, 12/10/2016.

Lisl Weynans has participated to the PhD defense of Andrea Filippini, Inria Bordeaux, 14/12/2016.

Angelo Iollo: Président du jury d'HDR de Heloise Beaugendre, Institut de Mathématiques de Bordeaux, université de Bordeaux, mars 2016.

Angelo Iollo: Membre Jury HDR de Laurent Cordier, Institut P', université de Poitiers, novembre 2016.

Angelo Iollo: Membre du Jury de thèse de Loic Lacouture « Modélisation et simulations de mouvement de structures fines » département de mathématiques, juin 2016, Université Paris Sud.

Angelo Iollo: Président du jury de thèse de Olivier Gallinato, « Modélisation du processus cancéreux et méthodes super-convergentes de résolution de problèmes d'interface sur maillage cartésien », Institut de Mathématiques de Bordeaux, université de Bordeaux, novembre 2016,

10.3. Popularization

Lisl Weynans has co-organized the Journée "Filles et Maths, une équation lumineuse": may 11t 2016

Lisl Weynans has co-organized Journée Emploi Maths de l'Unité de Formation "Mathématiques et Interaction"

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Major publications by the team in recent years

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- [2] M. BERGMANN, A. IOLLO. *Modeling and simulation of fish-like swimming*, in "Journal of Computational Physics", 2011, vol. 230, n^o 2, pp. 329 - 348
- [3] M. BERGMANN, A. IOLLO. *Bioinspired swimming simulations*, in "Journal of Computational Physics", 2016, vol. 323, pp. 310 - 321
- [4] M. BERGMANN, A. IOLLO, R. MITTAL. *Effect of caudal fin flexibility on the propulsive efficiency of a fish-like swimmer*, in "Bioinspiration & Biomimetics", 2014, vol. 9, n^o 4, 046001
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Publications of the year

Articles in International Peer-Reviewed Journals

- [11] M. BERGMANN, A. IOLLO. *Bioinspired swimming simulations*, in "Journal of Computational Physics", 2016, vol. 323, pp. 310 - 321 [DOI : 10.1016/j.jcp.2016.07.022], <https://hal.inria.fr/hal-01405039>
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Invited Conferences

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